Effective action and the quantum equation of motion

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Received: 1 April 2004 / Published online: 2 July 2004 – © Springer-Verlag / Società Italiana di Fisica 2004

Abstract. We carefully analyze the use of the effective action in dynamical problems, in particular the conditions under which the equation $\frac{\delta\Gamma}{\delta\phi} = 0$ can be used as a quantum equation of motion and illustrate in detail the crucial relation between the asymptotic states involved in the definition of Γ and the initial state of the system. Also, by considering the quantum-mechanical example of a double-well potential, where we can get exact results for the time evolution of the system, we show that an approximation to the effective potential in the quantum equation of motion that correctly describes the dynamical evolution of the system is obtained with the help of the wilsonian RG equation (already at the lowest order of the derivative expansion), while the commonly used one-loop effective potential fails to reproduce the exact results.

1 Introduction

The effective action $\Gamma[\phi]$, the generating functional of the one-particle irreducible (1PI) vertex functions, is a very useful tool in quantum field theories. It is widely used in the analysis of their vacuum structure [1] (for more recent reviews see e.g. [2,3]) and its symmetries are often exploited in order to establish their renormalization properties [4]. For vanishing external sources, it satisfies the equation

$$\frac{\delta\Gamma[\phi]}{\delta\phi(\mathbf{x},t)} = 0, \tag{1}$$

sometimes referred to as the quantum equation of motion, the quantum counterpart of the classical equation $\frac{\delta S}{\delta \phi} = 0$.

In fact, at the lowest order of the semiclassical expansion, $\Gamma[\phi]$ coincides with the classical action $S[\phi]$, and this property, when combined with (1), naively suggests that $\Gamma[\phi]$ should be regarded as the quantum action of the system, and (1) as the corresponding quantum dynamical equation. This interpretation, however, is correct only under certain conditions. Moreover, even when this interpretation applies, (1) in general cannot be straightforwardly related to any semiclassical expansion.

The dynamical content of (1) was already briefly discussed in [5], where a solid theoretical background to the work presented in [6] was provided along with the correction of some mistakes and misunderstandings. One of the purposes of the present paper is to present a more detailed description of the approach followed in [5], with the aim of clarifying the limits of applicability of this procedure.

As it is well known, an ansatz for $\Gamma[\phi]$ which is well suited for the applications is given by the gradient expansion, an expansion in powers of the field derivatives:

$$\Gamma[\phi] = \int d^4x \left(-V_{\text{eff}}(\phi) + \frac{Z(\phi)}{2} \partial_\mu \phi \partial^\mu \phi + Y(\phi) (\partial_\mu \phi \partial^\mu \phi)^2 + W(\phi) (\partial_\mu \partial_\mu \phi)^2 + \ldots \right) .$$
(2)

The lowest-order approximation, the so called local potential approximation (LPA), is obtained from (2) once we neglect the higher order derivatives and keep the wave function renormalization factor constant, i.e. field independent (without loss of generality we can choose Z = 1):

$$\Gamma[\phi] = \int d^4x \left(-V_{\text{eff}}(\phi(x)) + \frac{1}{2} \partial_\mu \phi(x) \partial^\mu \phi(x) \right) . \quad (3)$$

Within the LPA, (1) becomes

$$\partial^{\mu}\partial_{\mu}\phi = -\frac{\partial V_{\text{eff}}(\phi)}{\partial\phi},\qquad(4)$$

i.e. it takes the same form of the classical equation of motion where the classical potential is replaced by the effective potential.

This equation has been widely used in the past as the quantum equation of motion to describe the time evolution of the scalar field expectation value [7]. More recently, however, some of the limitations in the use of (4), and more generally of (1), as a dynamical equation have been

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noted [8] and a different formalism to deal with dynamical problems has been developed [8-10].

In the present paper we complement these previous studies and push the investigation of (4) a step further. We carefully analyze the limitations in the application of this equation to dynamical problems and show that there are physically relevant cases where it can be appropriately used to describe the evolution of expectation values. It will turn out that two points, overlooked in the past, play a crucial role: the correct consideration of the boundary conditions encoded in the definition of the effective action and the use of a non-perturbative approximation for the effective potential in (4).

Let us proceed now to our systematic analysis of the subtle points related to the use of (1) as a dynamical equation. As it will be clear in a moment, it is essential to specify (i) the framework in which (1) is derived, to avoid confusion on the physical meaning of ϕ ;

(ii) the choice of the boundary conditions (consistent with point (i)) associated to the differential equation (1);

(iii) the approximation in which $\Gamma[\phi]$ is computed, that has obviously to be well suited for the particular problem considered, in order to get physically meaningful results.

Concerning point (i), one has to be careful in considering ϕ as the field expectation value, because in general this is not true. The effective action $\Gamma[\phi]$ is the Legendre transform of W[J], the generator of the connected Green functions, defined by $e^{\frac{i}{\hbar}W[J]} = Z[J] = \langle 0, t = +\infty | 0, t = -\infty \rangle_J$. In the Schrödinger picture, the vacuum persistence amplitude, Z[J], can be explicitly written as

$$Z[J] = \langle 0|\hat{U}(+\infty, -\infty)|0\rangle$$

= $\langle 0|T\left(e^{-\frac{i}{\hbar}\int_{-\infty}^{+\infty} dt(\hat{H}-J(t)\hat{\varPhi}(\mathbf{x}))}\right)|0\rangle,$ (5)

where $\hat{U}(+\infty, -\infty)$ is the time evolution operator in the presence of the source J, and $|0\rangle$ is the ground state of \hat{H} , the Hamiltonian of the system. From (5), and from the definition of the classical field, $\phi(\mathbf{x}, t) = \frac{\delta W[J]}{\delta J(\mathbf{x}, t)}$, we immediately see that

$$\phi(\mathbf{x},t) = \frac{\langle -,t | \hat{\varPhi}(\mathbf{x}) | +, t \rangle}{\langle -,t | +,t \rangle}, \tag{6}$$

where

$$\langle -,t| = \langle 0|\hat{U}(+\infty,t) \text{ and } |+,t\rangle = \hat{U}(t,-\infty)|0\rangle.$$
 (7)

Clearly $|+, t\rangle$ and $|-, t\rangle$ are (in general) different states. As a consequence, $\phi(\mathbf{x}, t)$ is not (in general) a diagonal matrix element of the quantum field $\hat{\Phi}(\mathbf{x})$. Moreover it may be complex-valued. This is not surprising as Γ generates the 1PI vertex functions that are in general complex quantities satisfying causal (Feynman) boundary conditions. Only for particular choices of the external source J can we have $|+, t\rangle = |-, t\rangle$; under these conditions, (1) describes the dynamical evolution of the field expectation value of $\hat{\Phi}$.

Effective actions defined according to (5) are called Schwinger–De Witt (or "in–out") effective actions [11]. They incorporate boundary conditions that are appropriate to problems where the transition from asymptotic states in the past to asymptotic states in the future is considered (as is the case of a scattering process). In passing we note that more general definitions of "in–out" effective actions can be obtained if the $|0, t = -\infty\rangle$ and $|0, t = +\infty\rangle$ asymptotic states are replaced by more general $|in\rangle$ and $|out\rangle$ states, i.e. by more general asymptotic boundary conditions.

A functional formalism that is in general appropriate to dynamical problems is the so called "in–in" or closed-timepath formalism [12–14], where one can construct "in–in" effective actions that generate the dynamical evolution of expectation values. This formalism is the one most largely used nowadays in the applications to inflationary cosmology.

In this paper, however, we shall not deal with this latter approach and its most recent developments. Our aim is rather to show that, under certain conditions, we can still define an equation of motion in the in–out formalism.

In view of the fact that (1) is sometimes used as the quantum counterpart of the classical equation of motion, this problem is certainly worth to study.

Even in those cases where this formalism can be properly employed, however, we still have to face the problem mentioned in point (ii). Equation (5) contains two asymptotic conditions at the initial $(t = -\infty)$ and final $(t = +\infty)$ times. These conditions are encoded in the definition of the effective action itself, as well as in the definition of the classical field (the argument of Γ). It is then clear that we cannot freely choose certain boundary conditions for the field and its derivatives at a given initial time $t = t_0$, together with a "physically convenient" form for the (functional) wave packet of the system at the same time, and then evolve the expectation value of the quantum field according to (1). In fact arbitrary initial conditions for ϕ and for the wave packet in general are not compatible with the asymptotic conditions that enter the definition of Γ .

In the following, we provide arguments showing that, by considering a specific set of initial conditions for the expectation value of the field and of its derivatives, it is possible to find the form of the initial (i.e. at $t = t_0$) wave packet that is compatible with the asymptotic conditions encoded in the definition of the effective action and whose dynamical evolution is governed by (1). Our arguments will be strongly supported by the numerical results that we shall obtain for the dynamical evolution of the position operator expectation value in the quantum-mechanical double-well potential problem. In this case we are also able to consider the exact dynamical evolution with the help of the timedependent Schrödinger equation, so that we can compare the results obtained with (1) with the exact ones. As we shall see, when the initial wave packet is chosen according to our criterion, we find excellent agreement between the two results.

We have found it convenient to investigate the question of the determination of the initial wave packet within the framework of the variational definition of the effective action [15], that is the generalization to the time-dependent case of the well-known variational definition of the effective potential [16]. The effective action $\Gamma[\phi]$ is obtained through the extremization of a certain functional of two (a priori) different states, called $|\psi_+, t\rangle$ and $|\psi_-, t\rangle$, under the constraint that $\langle \psi_-, t | \hat{\Phi}(\mathbf{x}) | \psi_+, t \rangle = \phi(\mathbf{x}, t)$ (see next section).

Finally we come to point (iii) and to the problem of the approximations employed to compute the effective action and effective potential. The most simple approximation of Γ is given by the LPA, i.e. by (3), and the most straightforward approximation of the effective potential $V_{\rm eff}$ is given by the one-loop potential V_{11} . This last approximation however presents a serious drawback. The exact effective potential (actually the effective action) is a convex function of its argument [2, 17, 18]. However, when the classical (bare) potential is not convex (these are the physically most interesting cases), at any finite order of the loop expansion the approximated effective potential does not enjoy this fundamental property. Alternative non-perturbative methods of computing the effective action and potential, though, such as lattice simulations [19], variational approaches [20], or suitable averages of the perturbative results [21], provide the proper convex shape. In addition to the methods quoted above, a non-perturbative convex approximation to the effective potential, $V_{\rm RG}$, is found within the framework of the wilsonian renormalization group (RG) equation [22–26]. We have computed the effective potential with the help of this RG equation and then inserted $V_{\rm RG}$ in (4). The comparison of the results obtained with (1) with those obtained with the help of the time-dependent Schrödinger equation shows that $V_{\rm RG}$, because of its non-perturbative features, provides an excellent approximation for the correct "quantum potential" to be used in the "quantum equation of motion". For completeness we will also check the inadequacy of V_{11} to describe non-perturbative regimes with our equations of motion.

The plan of this paper is as follows. In Sect. 2 we briefly illustrate the basic formalism employed in the following. In Sect. 3 the central argument concerning the validity of (1) is discussed, while its application to the harmonic oscillator and to the double-well potential are respectively addressed in Sects. 4 and 5. The former example is treated analytically whereas the latter is solved by a numerical analysis. Section 6 contains the summary and outlook.

2 Variational definitions of $\Gamma[\phi]$ and $V_{ m eff}(\phi)$

To set up the tools of the following analysis, we briefly review in this section the variational principles that lead to the definitions of the effective action and the effective potential, referring to [15,16] for details. According to [15] the effective action is the stationary, time-integrated matrix element of $i\partial_t - \hat{H}$

$$\Gamma[\phi] = \int_{-\infty}^{+\infty} \mathrm{d}t \langle \psi_{-}, t| \left(\mathrm{i}\partial_{t} - \hat{H}\right) |\psi_{+}, t\rangle, \qquad (8)$$

where the right-hand side is stationary when the two timedependent states $|\psi_{\pm}, t\rangle$ are varied arbitrarily and independently, but with the two constraints

$$\langle \psi_{-}, t | \hat{\varPhi}(\mathbf{x}) | \psi_{+}, t \rangle = \phi(\mathbf{x}, t)$$
 (9)

and

$$\langle \psi_{-}, t | \psi_{+}, t \rangle = 1, \tag{10}$$

and with the asymptotic boundary conditions

$$\lim_{t \to \pm \infty} |\psi_{\pm}, t\rangle = |0\rangle, \tag{11}$$

where $|0\rangle$ is the ground state of \hat{H} .

This variation, together with the constraints (9) and (10), is translated into the equations

$$\left(\mathrm{i}\partial_t - \hat{H} + \int \mathrm{d}^3 \mathbf{x} \ J(\mathbf{x}, t) \hat{\varPhi}(\mathbf{x}) \right) |\psi_+, t\rangle = w(t) |\psi_+, t\rangle$$
(12)

$$\left(\mathrm{i}\partial_t - \hat{H} + \int \mathrm{d}^3 \mathbf{x} \ J(\mathbf{x}, t) \hat{\varPhi}(\mathbf{x}) \right) |\psi_-, t\rangle = w^*(t) |\psi_-, t\rangle,$$
(13)

where $J(\mathbf{x}, t)$ and w(t) are the Lagrange multipliers that implement the two constraints (9) and (10). The relation between the couple of states $|\psi_{\pm}, t\rangle$ and $|\pm, t\rangle$, introduced in (7), is shown in [15]. They are related by a phase factor given by the time integral of the Lagrange multiplier w(t).

If we limit ourselves to considering constant (in space and time) field configurations, the effective action is reduced (see (3)) to the effective potential, the generator of the 1PI graphs with vanishing external momenta:

$$\Gamma[\phi]|_{\phi=\text{const.}} = -V_{\text{eff}}(\phi) \int \mathrm{d}^4 x.$$
 (14)

As is well known, $V_{\text{eff}}(\phi)$ can be obtained by minimizing the expectation value of the Hamiltonian among the normalized time-independent states which have a field expectation value equal to ϕ [16], i.e.

$$V_{\rm eff}(\phi) = \min_{\psi} \langle \psi | \hat{H} | \psi \rangle, \tag{15}$$

with the states $|\psi\rangle$ subject to the constraints

$$\langle \psi | \hat{\varPhi}(\mathbf{x}) | \psi \rangle = \phi \tag{16}$$

and

$$\langle \psi | \psi \rangle = 1. \tag{17}$$

The constrained minimum condition in (15) generates the time-independent Schrödinger equation for a modified Hamiltonian:

$$\left(\hat{H} - J \int \mathrm{d}^3 \mathbf{x} \,\,\hat{\varPhi}(\mathbf{x})\right) |\psi\rangle = E |\psi\rangle,\tag{18}$$

where again J and E are the Lagrange multipliers associated to the two constraints (16) and (17). As is clear from (15), the ground state(s) of \hat{H} , which is (are) obtained by solving (18) with J = 0, is (are) associated to the minimum (minima) of $V_{\text{eff}}(\phi)$. Except for very few cases, the exact form of the effective action cannot be determined, and we have to resort to some approximation. A typical ansatz for Γ , very appropriate for our following considerations, is the gradient expansion, an expansion in terms of the field derivatives. Suitable approximations are obtained by considering truncations to a given order. Although in the applications we shall limit ourselves to considering the LPA (see Sects. 4 and 5), which is the lowest order in this expansion and is the approximation typically adopted in dynamical problems, the considerations that follow do actually apply to any order of the expansion (see next section).

3 The quantum equation of motion

We have already noted that the classical field $\phi(\mathbf{x}, t)$ (the argument of Γ) is not in general a diagonal matrix element, i.e. it is not the expectation value of the quantum field $\hat{\Phi}$ in a given state. However, as we shall see at the end of this section, under certain conditions the two states $|\psi_+, t\rangle$ and $|\psi_-, t\rangle$ of (8) coincide: $|\psi_+, t\rangle = |\psi_-, t\rangle = |\psi, t\rangle$, in which case $\phi(\mathbf{x}, t)$ is the expectation value of $\hat{\Phi}(\mathbf{x})$ in $|\psi, t\rangle$. For the moment we assume that we are under these conditions.

Let us now consider the differential equation for $\phi(\mathbf{x}, t)$, (1), once the effective action is approximated with a derivative expansion truncated at the order m, where 2m indicates the highest number of field derivatives (in the approximation considered in (3), it is m = 1). In order to get a unique solution of (1) in the time interval $[t_0, t_1]$ (where t_1 is arbitrarily chosen), we need 2m boundary conditions, which we can fix for instance on the manifold $t = t_0$, with t_0 chosen as the initial time for the evolution of ϕ .

To make contact with the variational principle discussed in Sect. 2, we have to consider the evolution of $\phi(\mathbf{x}, t)$ from $t = -\infty$ to $t = +\infty$, and therefore we must provide $\phi(\mathbf{x}, t)$ also in the time intervals $] - \infty, t_0]$ and $[t_1, +\infty]$. We can choose the function $\phi(\mathbf{x}, t)$ in these intervals arbitrarily, provided the asymptotic conditions in (11) and the proper matching of this function with the unique solution of (1) in the interval $[t_0, t_1]$ at the times t_0 and t_1 are taken into account. Once the function $\phi(\mathbf{x}, t)$ is assigned in the whole range $] -\infty, +\infty[$, the constraint on the right-hand side of (9) is defined and we are therefore able to implement the variational principle and to determine the corresponding source, which we indicate with $\overline{J}(\mathbf{x}, t)$, as well as the state $|\psi_+, t\rangle = |\psi_-, t\rangle = |\psi, t\rangle$.

We note in passing that the source $J(\mathbf{x}, t)$ can also be obtained from its well-known relation with the functional derivative of the effective action

$$\frac{\delta\Gamma[\phi]}{\delta\phi(\mathbf{x},t)} = J(\mathbf{x},t). \tag{19}$$

Equation (19) is the generalization of (1), when a source, linearly coupled to the field, is turned on. Obviously the source $J(\mathbf{x}, t)$ associated to the field $\phi(\mathbf{x}, t)$ considered above must vanish in the range $[t_0, t_1]$.

So, on the basis of the variational principle, we conclude that there is only one state $|\psi, t\rangle$ that is associated to the

specific function $\phi(\mathbf{x}, t)$ introduced above, and in particular that at $t = t_0$ the boundary conditions considered for the time evolution of the field are in fact related to $|\psi, t_0\rangle$. This is an important point because, as mentioned in the Introduction, if the constraints on the variational principle (see (9), (10) and (11)) are neglected, one can in general find more than one normalized state that is compatible with the set of boundary conditions fixed at t_0 . However, among these states, only $|\psi, t\rangle$ is truly related to the effective action and therefore to the full evolution of $\phi(\mathbf{x}, t)$ in the time interval $] - \infty, +\infty[$.

We can now understand what we have already anticipated in the Introduction concerning the applications. In a typical cosmological application the effective action is truncated as in (3), a convenient form of the wave packet at the initial time $t = t_0$ (typically gaussian) is taken, and the initial values for the expectation value of the scalar field ϕ and of its first time derivative are usually taken to be $\phi = \text{constant}$ and $\dot{\phi} = 0$. On the basis of the previous considerations, we easily understand that the time evolution of ϕ is not always related to the time evolution of the wave packet that has been considered, or, in other words, $\phi(\mathbf{x}, t)$ need not be the mean value of $\hat{\Phi}(\mathbf{x})$ in $|\psi, t\rangle$.

Our main problem is then the determination of $|\psi, t_0\rangle$, so that we can have a direct physical interpretation of the function $\phi(\mathbf{x}, t)$ as the time evolution of the expectation value of the field for that particular state. Even though it is certainly not easy to find a solution to our problem for generic boundary conditions, we expect that under certain circumstances it should be possible to determine $|\psi, t_0\rangle$. In the following we consider a case, which is relevant to the physical applications (see above), where $|\psi, t_0\rangle$ can be found. Namely we take at $t = t_0$ a constant field $\phi(\mathbf{x}, t_0) =$ ϕ_0 with vanishing derivatives up to the (2m)th order. Our goal is now to identify the state $|\psi, t_0\rangle$ defined through the variational principle.

To this end we consider a different physical problem, namely the case in which, for $t > t_0$, the field ϕ is a constant: $\phi = \phi_0$. For this new problem and for $-\infty < t < t_0$, the source J has to be equal to the one of the previous case $(J = \overline{J}(\mathbf{x}, t))$, while for $t > t_0$, J is given by the constant J_0 , which corresponds to ϕ_0 . This constant is obviously fixed by the condition

$$\left. \frac{\delta \Gamma[\phi]}{\delta \phi} \right|_{\phi = \phi_0} = J_0. \tag{20}$$

With this assignment for the source J, the solution of (12) for $t > t_0$ must be the time-independent state

$$|\psi(J_0)\rangle = |\psi, t_0\rangle. \tag{21}$$

In fact in this case (12) becomes

$$\left(\hat{H} - J_0 \int d^3 \mathbf{x} \ \hat{\Phi}(\mathbf{x}) - E_0\right) |\psi(J_0)\rangle = 0, \qquad (22)$$

where $w(t) = -E_0$ is now a time-independent constant, and the two constraints in (9) and (10) are

$$\langle \psi(J_0) | \Phi(\mathbf{x}) | \psi(J_0) \rangle = \phi_0, \quad \langle \psi(J_0) | \psi(J_0) \rangle = 1.$$
 (23)

Clearly this is nothing else than the time-independent variational principle that defines the effective potential (see (14)–(18)). We then have found that the state $|\psi, t_0\rangle =$ $|\psi(J_0)\rangle$ we were looking for is nothing but the normalized time-independent state that provides the minimum expectation value of the Hamiltonian \hat{H} among the normalized states with field expectation value equal to ϕ_0 .

There is one main assumption behind this result, and it concerns the source J. In fact, for our purposes, we have considered two different sources, which are both equal to $\overline{J}(\mathbf{x},t)$ in the range $-\infty < t < t_0$, whereas for $t > t_0$ one is vanishing while the other is a non-vanishing constant $J = J_0$. Note that, by construction, $J_0 = \overline{J}(\mathbf{x}, t_0)$. Therefore in the former case the source is discontinuous at $t = t_0$ and we are assuming that this has no consequences on the determination of the solution of the time-dependent Schrödinger equation. This discontinuity could be replaced with a sharp but still continuous change of the function Jaround $t = t_0$, but again we would have to assume that this has no consequences on the determination of the state.

Finally, let us come back to the important question, mentioned at the beginning of this section, that at least in some cases the effective action (or an approximation of it) can be obtained as a diagonal matrix element, i.e. in (8) we have $|\psi_{-}, t\rangle = |\psi_{+}, t\rangle$. We now argue that this should be the case when the motion of the field ϕ in the time interval $[t_0, t_1]$, i.e. the time interval where the motion of ϕ is governed by (1) plus a set of boundary conditions, is periodic. Suppose that this time interval covers n periods (let us call Δt the period), i.e. that $t_1 = t_0 + n \Delta t$. Then, at time $t = t_1$, the field ϕ and its derivatives take the same values as at $t = t_0$.

Now we can obviously make a shift on the time axis without changing the physics and take the point t = 0 to be symmetric with respect to t_0 and t_1 , i.e. $-t_0 = t_1 = \overline{t}$ in the new frame. Let us now choose J in (12) to be symmetric for time reflection, namely J must be taken in such a way that the ground state at $t = -\infty$ is driven onto $|\psi, -\overline{t}\rangle$ at $t = -\overline{t}$ (and as before we indicate this particular source as $\overline{J}(\mathbf{x}, t)$ with $-\infty < t < -\overline{t}$), then J = 0 within the range $[-\overline{t}, \overline{t}]$ (in this interval ϕ covers n periods), and, for $\overline{t} < t < +\infty$, the source is turned on symmetrically, i.e. $J(\mathbf{x}, t) = \overline{J}(\mathbf{x}, -t)$.

Clearly, with such a choice, the evolution of the two states in (12) and (13) is symmetric for time reversal and therefore equal, i.e. $|\psi_+, t\rangle = |\psi_-, t\rangle$. It must be noticed that the class of periodic motions of ϕ obviously includes the case of constant ϕ (i.e. the case associated to a constant non-vanishing source), which was also considered above.

The conclusion of this section is that, at least for those cases in which we consider a truncated derivative expansion of the effective action which gives rise to a periodic dynamical evolution of ϕ , this latter quantity has the meaning of the expectation value of the field operator, and the associated quantum state, at some particular time $t = t_0$, can be identified with the state that defines the effective potential through the static variational principle (see (14)–(18)).

4 An application. The harmonic oscillator

We now discuss a simple application of the results presented in the previous section. As in [15], we consider a trivial field theory (in one time and zero space dimension), namely the case of a one-dimensional harmonic oscillator whose Hamiltonian is ($\hbar = m = 1$)

$$\hat{H} = \frac{\hat{P}^2}{2} + \frac{\omega^2 \hat{Q}^2}{2} - \frac{\omega}{2}.$$
(24)

The term $-\frac{\omega}{2}$ has been added in order to have a vanishing vacuum energy.

In this case it is known that the effective action Γ coincides with the classical action S. In [15] this result has been recovered by means of the variational principle, which we illustrated in Sect. 2, and the explicit solutions of (12) and (13) for a generic source function J(t) have been shown to be

$$\langle Q|\psi_{+},t\rangle = \langle Q|\psi_{-},t\rangle$$

$$= \left(\frac{\omega}{\pi}\right)^{1/4} \exp\left\{-\frac{\omega}{2}(Q-q)^{2} - \mathrm{i}\dot{q}(Q-q) - \frac{\mathrm{i}q\dot{q}}{2}\right\},$$
(25)

with

$$q(t) = \langle \psi_{-}, t | \hat{Q} | \psi_{+}, t \rangle = \frac{i}{2} \int_{-\infty}^{+\infty} dt' \ J(t') \ e^{-i\omega|t-t'|}.$$
 (26)

Also, the Lagrange multiplier w(t) turns out to be w(t) = J(t)q(t).

From (25) we see that $|\psi_+, t\rangle = |\psi_-, t\rangle$ as was expected because of the periodicity of the motion of q for the harmonic oscillator effective action. Moreover, we see that the right-hand sides of (25) and (26) are totally determined once the source J is given.

In addition we show a concrete realization of the procedure illustrated in Sect. 3. In fact, we derive from the effective action the equation of motion for q(t) which is equal to the classical one (being in this case $S[q] = \Gamma[q]$) and we therefore have the typical solution

$$q(t) = A \cos(\omega t + \omega \tau), \qquad (27)$$

where the constant τ is fixed by the boundary conditions. By taking

$$\tau = \frac{n\pi}{\omega} \tag{28}$$

with *n* integer and $t_0 = -\tau$ (where t_0 is defined in Sect. 3), we get $q(t_0) = A$ and $\dot{q}(t_0) = 0$. Moreover q(t) covers *n* periods in the time range $[-\tau, \tau]$ and so $q(\tau) = A$ and $\dot{q}(\tau) = 0$.

Our problem here is to find the source J(t) that drives q(t) from $q(-\infty) = 0$ (in fact as seen in Sect. 3, the quantity q at $t = \pm \infty$ must be the expectation value of the coordinate for the ground state of the harmonic oscillator, which is zero) to the value $q(-\tau) = A$. Then, after the interval $-\tau < t < \tau$ where J = 0 and q(t) has the mentioned periodic behavior, q must evolve from $q(\tau) = A$ to $q(+\infty) = 0$.

This source is

$$J(t') = A \ \omega \ e^{-\epsilon |t'|}$$
(29)
(-\overline < t' < -\tau) and (\tau < t' < +\infty),
$$J(t') = 0 \quad (-\tau < t' < \tau),$$
(30)

where ϵ is a small parameter, which eventually has to be sent to zero. In fact by inserting this particular source into (26), q(t), for $-\tau < t < \tau$ is given by

$$q(t) = \frac{i\omega A}{2}$$

$$\times \lim_{\epsilon \to 0} \lim_{T \to +\infty} \left\{ \int_{-T}^{-\tau} dt' e^{-i\omega t} e^{i\omega t'} e^{\epsilon t'} + \int_{\tau}^{T} dt' e^{i\omega t} e^{-i\omega t'} e^{-\epsilon t'} \right\}$$

$$= A \cos(\omega t + \omega \tau), \qquad (31)$$

where we have introduced the intermediate step of cutting the time integrals at a large time T > 0 and then taking the limit $T \to +\infty$, which will be helpful in the following calculations. The final result in (31), which is the desired solution introduced in (27), has been obtained with the help of

$$\exp(-i\omega\tau) = \exp(i\omega\tau), \tag{32}$$

which holds because of (28).

We also check the behavior of q(t) for $t \to +\infty$, as obtained from the source defined in (29) and (30). We therefore compute the integral in (26) by introducing as before the cutoff $\pm T$ for large (positive and negative) values of t' and putting t = T, and then taking the limits $T \to +\infty$ and $\epsilon \to 0$:

$$q(+\infty) = \frac{i\omega A}{2}$$

$$\times \lim_{\epsilon \to 0} \lim_{T \to +\infty} \left\{ \int_{-T}^{-\tau} dt' e^{-i\omega T} e^{i\omega t'} e^{\epsilon t'} + \int_{\tau}^{T} dt' e^{-i\omega T} e^{i\omega t'} e^{-\epsilon t'} \right\}$$

$$= \frac{i\omega A}{2}$$

$$\times \lim_{\epsilon \to 0} \lim_{T \to +\infty} \left\{ \frac{e^{-i\omega T}}{i\omega + \epsilon} e^{-i\omega \tau - \epsilon \tau} - \frac{e^{-i\omega T}}{i\omega - \epsilon} e^{i\omega \tau - \epsilon \tau} \right\} = 0.$$
(33)

Instead of taking the limit $T \to \infty$ in the last line of (33), we keep T fixed to a very large value due to the oscillating terms $\exp(-i\omega T)$ and perform the limit $\epsilon \to 0$. Then, by making use of (32), we find $q(+\infty) = 0$. The computation for $q(-\infty)$ is totally analogous and gives again $q(-\infty) = 0$.

Equations (31) and (33) provide the desired results for the source J(t) defined in (29) and (30). As noted in Sect. 3, there is a discontinuity in the function J(t) at the two points $t = \pm \tau$; however, in this particular example there is no consequence on the coordinate expectation value (and its derivatives), which are continuous at those points.

According to Sect. 3 we must also find a new source that determines a static coordinate expectation value, namely q(t) = A for $-\tau < t < \tau$. For this purpose, we retain the definition in (29) for large positive and negative times but, following the argument in Sect. 3, instead of (30), we now take $J = A \omega \exp(-\epsilon \tau)$ constant in the time interval $[-\tau, \tau]$ and this new source does not have any discontinuity points. Moreover in the two asymptotic regions the integrals for t'are equal to the ones performed above and we have only to compute the contributions in the region where the former source vanishes according to (30). Therefore, for $-\tau < t <$ τ , q(t) is given by (31) plus an additional term (note that, when performing an integral in this limited range $[-\tau, \tau]$ the term $\exp(-\epsilon\tau)$ in the new source will always tend to 1 for $\epsilon \to 0$ and it can therefore, for simplicity, be neglected from the beginning):

$$q(t) = A \cos(\omega t + \omega \tau) + \frac{i\omega A}{2} \int_{-\tau}^{\tau} dt' e^{-i\omega|t-t'|}$$
$$= A \cos(\omega t + \omega \tau) + \frac{A}{2} \left(2 - e^{-i\omega(t+\tau)} - e^{i\omega(t+\tau)}\right)$$
$$= A, \tag{34}$$

where again (32) has been used. This is exactly the required solution for q.

Finally, in order to check that q(t) vanishes asymptotically even with this source, we must check that the vanishing result in (33) is not modified. This time we have the additional contribution

$$q(+\infty) = \frac{\mathrm{i}\omega A}{2} \int_{-\tau}^{\tau} \mathrm{d}t' \,\mathrm{e}^{-\mathrm{i}\omega(T-t')}$$
$$= \frac{A\mathrm{e}^{-\mathrm{i}\omega T}}{2} \left(\mathrm{e}^{\mathrm{i}\omega\tau} - \mathrm{e}^{-\mathrm{i}\omega\tau}\right) = 0, \qquad (35)$$

which is vanishing because of (32). The same is valid for $q(-\infty)$.

5 The double-well potential

As a further test of the arguments presented in Sect. 3, we now consider the non-trivial case of the motion of a wave packet in a double-well potential. To follow the dynamical evolution of the position operator expectation value, we make use of (1) within the framework of the LPA (see (3)) for the effective action. The effective potential $V_{\rm eff}(q)$ is obtained with the help of the wilsonian RG equation (see below), which, as we mentioned before, gives a non-perturbative, convex, effective potential (for comparison also the one-loop effective potential will be considered at the end of this section). Again we fix for q and \dot{q} the two initial conditions

$$q(t_0) = q_0$$
 and $\dot{q}(t_0) = 0.$ (36)

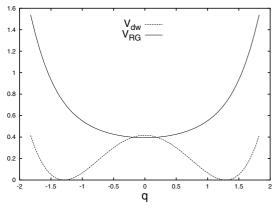


Fig. 1. $V_{\rm dw}(q)$ and $V_{\rm RG}(q)$ for $\lambda = 0.15$

Then, being again in the presence of a periodic motion, we are allowed to use (1) as an equation of motion for $q(t) = \langle \hat{Q} \rangle_t = \langle \psi, t | \hat{Q} | \psi, t \rangle.$

According to our arguments, the function q(t) derived by means of the above procedure should be equal to the one obtained by solving the time-dependent Schrödinger equation with the form of the initial wave packet fixed by (22). In fact we have numerically solved the latter problem with the initial conditions given by (22); for comparison, we also considered the evolution of an initial gaussian wave packet that is often used in the applications¹.

When we compare these results with the one obtained within the framework of the effective action formalism, we see that, given the initial conditions (36), (1) (together with (3)) provides a very accurate description of the dynamical evolution of q(t), if the initial state is chosen according to our criterion, i.e. with the help of (22). We also see that the (non-convex) one-loop effective potential, that is the approximation to V_{eff} considered in the applications, is inadequate to describe the dynamics of q(t).

In Fig.1 we have plotted the double-well potential $V_{\rm dw}(q)$, which we have written as $V_{\rm dw}(q) = -\frac{1}{2}q^2 + \lambda q^4 + \frac{1}{16\lambda}$, together with the effective potential $V_{\rm eff}(q)$, obtained by solving the RG equation [28–31]

$$\frac{\partial U_k(q)}{\partial k} = -\frac{1}{2\pi} \ln \left(1 + \frac{U_k^{''}(q)}{k^2} \right) \tag{37}$$

(here $U_k''(q)$ means $\frac{\partial^2 U_k(q)}{\partial q^2}$). Note that in this framework the classical double-well potential $V_{dw}(q)$ is nothing but the bare potential, i.e. the UV boundary condition for $U_k(q)$; also note that the effective potential $V_{\text{eff}}(q)$ is approximated by the solution of (37), once it has been integrated down to k = 0, i.e. once the quantum fluctuations have been taken into account: $V_{\text{eff}}(q) = V_{\text{RG}}(q) = U_{k=0}(q)$. Also, when (3) is inserted in (1), the quantum equation of motion for q(t) takes the form

$$\ddot{q} = -\frac{\mathrm{d}}{\mathrm{d}q} \, V_{\mathrm{eff}}(q) \,, \tag{38}$$

i.e. the dynamical evolution of q(t) is given by the classical equation of motion, being the classical potential replaced by V_{eff} , which, as discussed above, will be approximated by V_{RG} in our numerical analysis.

We now illustrate the above points by computing q(t)and $p(t) (= \dot{q}(t))$ for three different values of λ : 1.1, 0.15 and 0.07. We also choose the initial time as $t_0 = 0$, and the initial values of q and \dot{q} as follows: q(0) = 0.2 for $\lambda = 1.1$, q(0) = 0.5 for $\lambda = 0.15$, q(0) = 1.0 for $\lambda = 0.07$, and $\dot{q}(0) = 0$ for each value of λ .

According to our arguments, for such a choice of the initial values, (1) describes the time evolution of the expectation value q(t) related to the initial wave packet, which is obtained by solving the time-independent Schrödinger equation (see (22))

$$\left(-\frac{\hbar^2}{2m}\Delta + V_{\rm dw}(q) - Jq\right)\psi(q) = E_J\psi(q)\,,\qquad(39)$$

where, for each of the chosen initial values of q(t), $J = J(q_0)$ is computed with the help of the equation $\langle \psi_J | \hat{Q} | \psi_J \rangle = q_0$ (for notational convenience we have replaced q(0) by q_0).

Once the initial wave packet $\psi(q, 0)$ is obtained with the help of (39), $\psi(x, t)$ is obtained by solving the timedependent Schrödinger equation numerically, and the exact values of q(t) and p(t) are then computed. These results are compared with those obtained by solving (1).

As we already discussed in the Introduction, the boundary conditions that define the effective action are not appropriately taken into account in the applications of the effective action formalism to dynamical problems. Typically one associates a gaussian initial wave packet with the initial conditions (36). For this reason we have also considered the exact evolution of a gaussian wave packet, $\psi_g(q)$, chosen in such a way that its width is equal to that of the ground state of the harmonic approximation at the bottom of one of the two wells.

For each of the three values of λ considered, we present in the following figures the shape of the initial wave packets, $\psi_{J}(q)$ and $\psi_{g}(q)$, the expectation value of the position operator $\langle \hat{Q} \rangle_{t} = q(t)$ as a function of time, and the phase-space q-p diagram.

In Figs. 2 and 3 we present the results for the $\lambda = 1.1$ case. From Figs. 2b and 3 we see that the results obtained with $\psi_J(q)$ and $\psi_g(q)$ are almost the same (and that they are both well approximated by the results of (38)). As is clear from Fig. 2a, this is because, for this particular value of λ , $\psi_r(q)$ almost coincides with $\psi_J(q)$.

However, we shall now see that, when we consider other values of λ , corresponding to different heights of the potential barrier, the choice of the correct initial wave packet becomes crucial. Taking for instance $\lambda = 0.15$, we obtain two different shapes for $\psi_J(q)$ and $\psi_g(q)$ (Fig. 4a). It is not difficult to imagine that they have a different dynamical evolution, as can actually be seen from Figs. 4b and 5. The crucial result for our analysis is that (38), i.e. the LPA

¹ The RG flow equation for $V_{\rm RG}$ and time-dependent Schrödinger equation were solved with the help of the NAG routines [27]. These routines were also used to compute the mean values of \hat{Q} and \hat{P} .

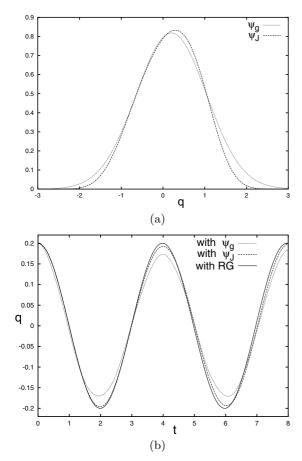


Fig. 2. The case $\lambda = 1.1$. **a** The initial wave packets $\psi_J(q)$ and $\psi_g(q)$. **b** The time evolution of q(t) as obtained from the Schrödinger equation with initial wave packets $\psi_J(q)$ and $\psi_g(q)$, and from (38) with the initial conditions given in the text

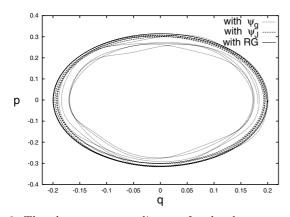


Fig. 3. The phase-space q-p diagram for the three cases considered in Fig. 2b ($\lambda = 1.1$)

of (1), gives a very good approximation to the time evolution of $\langle \hat{Q} \rangle$ when the initial state is $\psi_J(q)$ (see Fig. 5). This gives a very robust support to the arguments we have developed in Sect. 3.

As an additional example, we have considered the case $\lambda = 0.07$. Once more, Figs. 6 and 7 confirm that the effective action formalism, in particular the LPA we have considered in the present paper, actually describes the dy-

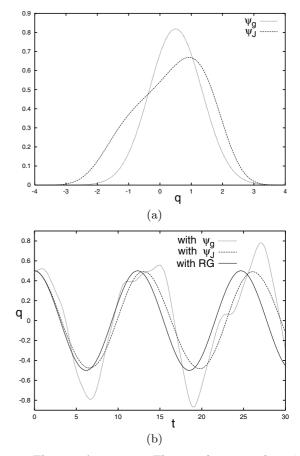


Fig. 4. The case $\lambda = 0.15$. **a** The initial wave packets $\psi_J(q)$ and $\psi_g(q)$. **b** The time evolution of q(t) as obtained from the Schrödinger equation with initial wave packets $\psi_J(q)$ and $\psi_g(q)$, and from (38), with the initial conditions given in the text

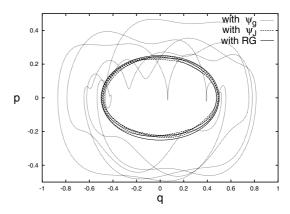


Fig. 5. The phase-space diagram for the three cases considered in Fig. 4b ($\lambda = 0.15$)

namical evolution of the expectation value of the position operator once the initial state is selected according to (39).

It is worth noting that, because of the initial conditions chosen for \dot{q} , the cases considered above describe tunnelling processes. Needless to say, a semiclassical expansion of Γ at the lowest order, i.e. the approximation $\Gamma = S$, would have been unable to describe these tunnelling processes. In fact, in this approximation, $V_{\rm eff} = V_{\rm dw}$.

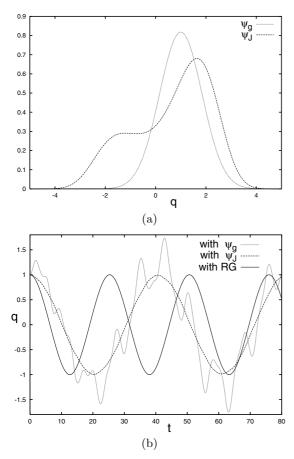


Fig. 6. The case $\lambda = 0.07$. **a** The initial wave packets $\psi_J(q)$ and $\psi_g(q)$. **b** The time evolution of q(t) as obtained from the Schrödinger equation with initial wave packets $\psi_J(q)$ and $\psi_g(q)$, and from (38) with the initial conditions given in the text

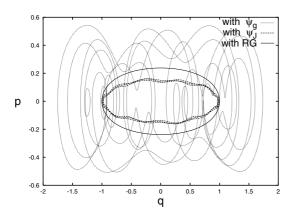


Fig. 7. The phase-space diagram for the three cases considered in Fig. 6b ($\lambda = 0.07$)

From the above results, it is clear that the trajectory of the gaussian wave deviates more and more from the correct result for decreasing values of λ , i.e. for larger quantum effects due to the tunnelling. Therefore it can be employed as an ansatz of the correct wave packet only for a specific range of the coupling λ and this is exactly what has been done in [5], where the results obtained with a gaussian wave packet are still accurate (as is the case for $\lambda = 1.1$ as considered above).

This is a clear indication that a semiclassical approximation to (1), which, for perturbatively small values of λ , would correspond to the periodic motion of an almost gaussian wave packet around one of the classical minima, is misleading. The trajectory obtained from (1) includes quantum effects that are neglected in a semiclassical approach.

Figure 7 needs one more comment. In fact for this smaller value of λ the phase-space q-p diagram obtained with the "correct" initial wave packet, even though it is still qualitatively well described by the phase-space diagram obtained with (38), shows a certain deviation from the latter. The reason for such a deviation has already been explained in [5] and has to be traced back to the approximation that we have used for Γ , the LPA. Actually, it was shown in [5] that the successive step in the derivative expansion of the effective action, i.e. the inclusion of the wave-function renormalization in (3), provides an improvement of the LPA results. Here we are concerned with different problems, and so no longer pursue this issue.

Before ending this section we would like to add a comment concerning the approximation of V_{eff} , namely the one-loop approximation $V_{\text{eff}} \sim V_{11}$. In Fig. 8a we show the one-loop effective potential versus the RG effective potential. As is well known, the one-loop potential does not enjoy the convexity property of the exact effective potential V_{eff} . Actually this is true at any finite order of the loop expansion for the effective potential. Moreover, in the region between the two inflection points of the classical potential, the oneloop potential develops an imaginary part; according to the usual interpretation [21], this signals the instability of the configurations in this region. In Fig.8a the real part of the potential is shown, which is the only part that is taken into account in dynamical problems.

As is well known, V_{11} can be obtained analytically by replacing $U_k^{''}$ by $U_A^{''}$ in (37) (remember that $U_A = V_{dw}$), and then performing the elementary integration from k = 0to $k = \Lambda$, i.e. by solving the RG flow equation in the independent-mode approximation. We thus obtain $V_{11} =$ $V_{dw} + \delta V_{11}$. Expanding in $\frac{1}{\Lambda}$ and neglecting *q*-independent terms, we can write the one-loop correction δV_{11} as

$$\begin{cases} \delta V_{11} = \frac{1}{\pi} \sqrt{V_{dw}''} \arctan \frac{\Lambda}{\sqrt{V_{dw}''}} + O\left(\frac{1}{\Lambda}\right) \\ \text{for } |x| > \frac{1}{\sqrt{12\lambda}}, \\ \delta V_{11} = -\frac{1}{2\pi} \frac{V_{dw}''}{\Lambda} + O\left(\frac{1}{\Lambda^2}\right) + \frac{i}{2} \sqrt{-V_{dw}''} \\ \text{for } |x| < \frac{1}{\sqrt{12\lambda}}. \end{cases}$$
(40)

From the above equations we see that, in the region $|x| < \frac{1}{\sqrt{12\lambda}}$, $\mathcal{R}(\delta V_{11})$ vanishes with $\Lambda \to \infty$. A comparison of Fig. 8a with Fig. 1 also shows that, within this inner region, V_{11} is practically equal to V_{dw} . This is an example of the well-known fact that the loop expansion cannot change the concavity of V_{dw} .

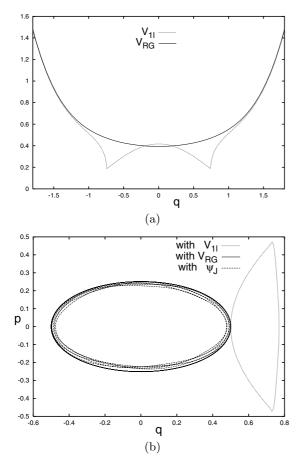


Fig. 8. a The one-loop (non convex) effective potential compared with the RG (convex) one. b The phase-space diagrams obtained from (38) with V_{eff} approximated by V_{11} and V_{RG} , for a motion with q(0) = 0.5 corresponding to an energy below the potential barrier. Differently from V_{RG} , V_{11} completely fails in describing the tunnelling. In **a** and **b** it is $\lambda = 0.15$

It is clear that for the kind of problems we have considered in this section, namely for tunnelling processes, the one-loop effective potential V_{11} is as inadequate as the classical potential V_{dw} to approximate V_{eff} in (38). This is illustrated in Fig. 8b, where it is shown that for an initial energy below the energy barrier the motion is obviously confined within one well. According to the results of the semiclassical expansion, we can actually state that at no finite order of this expansion can these phenomena be described by replacing the semiclassical effective potential in (38). Instead they are perfectly well described by the solution of (37), V_{RG} , which is only the lowest-order approximation to V_{eff} of a different expansion, namely the gradient expansion.

In order to push this comparison a step further, we have also considered a motion with energy above the potential barrier. Naturally, in this case, by replacing V_{11} in (38) we obtain a solution that, as is the case for $V_{\rm RG}$, explores the whole allowed region in position space. However, as is shown in Fig. 9, the correct description of the motion is again given by $V_{\rm RG}$ and not by V_{11} .

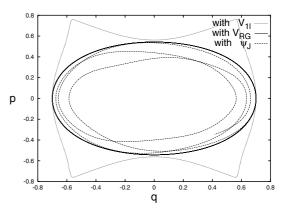


Fig. 9. The phase-space diagrams obtained from (38), with V_{eff} approximated respectively by V_{11} and V_{RG} , for a motion with q(0) = 0.7 corresponding to an energy above the potential barrier. Even if now also V_{11} allows the whole q-region to be explored, again we see that the motion is quite well described by V_{RG} and not by V_{11} . Here we have taken $\lambda = 0.25$

6 Summary and outlook

In the present work we have shown that in order to make use of the equation $\frac{\delta\Gamma[\phi]}{\delta\phi(\mathbf{x},t)} = 0$ ((1) in the text) as a "quantum equation of motion", attention has to be paid to a certain number of important issues.

First of all we need to make sure that we are under conditions such that the argument of Γ , the classical field $\phi(\mathbf{x}, t)$, is actually the expectation value of the quantum operator $\hat{\Phi}(\mathbf{x})$ in a given state $|\psi, t\rangle$, which is not always the case.

Once we are under these conditions, we have shown that the asymptotic $|\text{in}\rangle$ and $|\text{out}\rangle$ states that enter the definition of the effective action have to be taken appropriately into account in the determination of the initial wave functional $\Psi[\phi(\mathbf{x}, t_0)]$ associated with the motion of $\phi(\mathbf{x}, t)$. More precisely, by considering a derivative expansion for Γ , we have argued that it is possible to determine uniquely the initial state $\Psi[\phi(\mathbf{x}, t_0)]$ from the boundary conditions for the motion of $\phi(\mathbf{x}, t)$, assigned for instance on a given manifold $t = t_0$ (initial time), together with the asymptotic conditions encoded in the $|\text{in}\rangle$ and $|\text{out}\rangle$ states.

For initial conditions that are particularly important in the applications, namely the case of constant initial ϕ and vanishing derivatives of ϕ at $t = t_0$, we have been able to show that the initial (functional) wave packet obeys a modified time-independent *Schrödinger* equation, actually the equation that allows the definition of the effective potential.

Finally we have shown that, in the framework of the LPA for Γ , where the quantum equation of motion is obtained by the classical equation of motion once the classical potential is replaced by the effective potential, a reliable approximation to the effective potential comes from the solution of the corresponding wilsonian RG equation; instead, the one-loop effective potential, and more generally any finite-order approximation to the loop expansion for V_{eff} , fails to describe the dynamics of $\phi(\mathbf{x}, t)$.

All the above points have been illustrated by considering quantum-mechanical examples. After a brief application of these results to the simple case of the harmonic oscillator, which confirmed our arguments, we have considered the case of a double-well potential. The nice feature of considering a quantum-mechanical example is that we have the possibility to compute also the dynamical evolution of the wave packets with the time-dependent Schrödinger equation, i.e. we can compare our results with exact results. The cases we have investigated all confirm the correctness of our conjectures.

One point that was not considered in the present work concerns the possible extension of these results to the case of higher orders in the derivative expansion of Γ . It would also be interesting to investigate the impact of the presence of non-local terms in Γ . We plan to investigate this point in future work.

Naturally our ultimate goal is to apply our results in a QFT context where, as we cannot solve the quantummechanical (Heisenberg or Schrödinger) equations exactly, we really need to have sensible approximation schemes. We hope that our results can help in this direction.

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